

1 Theory of Electron Phenomena in Deformed Crystals

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1.0.1 Abstract

On this article there are presented the main results of the theory of electron phenomena in an unordered condensed matter that can be described as an inhomogeneously deformed crystalline lattice with dislocations. The one-electron effective Hamiltonian is derived by introducing a new basis for the expansion of the sought functions. It allows to overcome the difficulty of the discontinuity of the displacement field. The same method is used for the derivation of the equations for eigentone of a deformed crystal, and the equations of the theory of dynamical scattering of electrons by it. The general problem of the description of the totality of electron states in a deformed crystal is discussed, and some new solutions describing localized electron or vibration states are obtained. There is derived and researched the equation of an electrical field generated by the deformation in a crystal with consideration for the interaction of electrons and ions by the self-consistent field theory. The tensor kinetic coefficients are obtained, which are proportional to the deformation tensor. Such kind of these coefficients can explain some experimental effects. The appearing of the local superconducting regions and the subsidiary solenoidal current that is generated by a transport one in a deformed superconductor is considered. The behavior and properties of the Abrikosov's vortex in anisotropic and/or deformed superconductors are researched. In more detail this theory has been published in the monograph by the same author of the same title in Russian.

1.1 1. Account of Deformed Crystal

In the title of this article as the "deformed crystal" the unordered solid-state substance is named. In this crystal the equilibrium sites of atoms form a lattice that can be described as a inhomogeneously deformed crystalline lattice with dislocations. The electron potential energy differs from the periodic function of coordinates in other way than in a crystal disordered by localized defects, *e. g.*, interstitial or substitutional impurities. In the site representation these cases can be considered as alternative limiting cases, because the localized defects are described by the diagonal disorder, but a deformation changes the non-diagonal hamiltonian elements and makes them dependent on site coordinates, and not only on their differences. Electron phenomena in non-ideal crystals with localized defects have been investigated in a very large number of experimental and theoretical works. Deformed crystals have been investigated poorly, and

the author devoted many years to their systematic investigations based on the unified method of attack. This article is an announcement of the main results of this research. In more detail this theory has been published in the monograph [1] in Russian.

The proposed method of attack is applicable in the case, when the difference of the deformed crystal from the ideal one can be described in the most part of area by some small and smooth function of coordinates. We shall name functions "smooth", when their variation on a distance of the order the ideal crystal lattice constant is negligible. The other definition of the smooth function: its Fourier-image is negligible outside of the vicinity of the origin of coordinates of the reciprocal space with the radius much smaller than the characteristic dimension of the Brillouin zone of the corresponding ideal crystal. Functions that describe the crystal deformation are introduced using Lagrange's coordinates. Let us conceive that before to be deformed the ideal crystal lattice was rigidly connected with a continuum, in which the Cartesian coordinate net of lines is embedded. When the deformation is performed, the lines of this net are distorted and transformed into the net of coordinate lines the Lagrange's curvilinear coordinate system. The coordinates in this system and the Cartesian coordinates that are independent on the deformation (they are named Euler's) are connected by the following equation:

$$\mathbf{x} = \mathbf{y} + \mathbf{u}(\mathbf{y}).$$

(1) Here \mathbf{x} is the Euler's coordinate, \mathbf{y} is the Lagrange's coordinate, and $\mathbf{u}(\mathbf{y})$ is the displacement field. In the cases when the displacements are small and are unambiguously defined this field can be used for the describing of the deformation. As this takes place, the displacements can be considered as small parameters of the perturbation for the hamiltonian of an electron in the periodic field. This approach is commonly employed in the theory of the electron-phonon interaction, in which deformation is generated by vibrations of atoms near the sites of the ideal lattice. In the case of static deformation the displacements are usually non-small, and when the deformation is generated by topological defects, *i. e.* by dislocations, they can't be described by a continuous unambiguous field. Then for the investigation of the electron-deformation interaction it is useful to describe the deformation by the field of the distortion tensor \mathbb{W} that is introduced by using the differentials of the Euler's and Lagrange's coordinates:

$$d\mathbf{x} = (\mathbb{I} + \mathbb{W}) d\mathbf{y}, \quad i. e. \quad dx_i = (\delta_{ij} + w_{ij}) dy_j.$$

This underlines the need for the general case to take precisely the distortion tensor, but not its symmetric term, *i. e.* deformation, as it was made elsewhere. The point is that the deformation describes the change of the shape of a cubic volume element, and the antisymmetric term of the distortion tensor describes its turning. It is obvious that, when the no-deformed crystal was anisotropic, the local turning is also significant for the properties of the deformed crystal. The distortion tensor is always an unambiguous field. It is dimensionless, small and smooth in the most part of the crystal volume. It can have singularities in some points and dislocation lines, and then takes large values in the vicinities of these singularities. If these areas would be eliminated from the consideration, the distortion tensor can be taken as the useful phenomenological parameter.2.

1.1.1 2.1. Short History of Problem

The fundamental method of studying electron states in a deformed crystal that consists of neutral and short-range ions, which is used in the monograph [1] and elsewhere, is the method of the effective hamiltonian. It was first put forward by S. I. Pecar [2], and next was developed and justified in many works, from which the works by J. M. Luttinger and W. Kohn [3,4] are best suited to our purpose. The fundamental task of this method is the construction of the operator, smooth eigenfunctions of which are some eigenfunctions of the initial hamiltonian with averaged short-wave variations, and the corresponding eigenvalues describe the part of the energy spectrum. This effective hamiltonian usually involves the kinetic energy and the smooth term of the potential energy of the initial hamiltonian. The kinetic energy is the dependence of the energy on quasi-momentum for the considered band (the law of dispersion). in which the quasi-momentum is changed by the kinematic momentum operator. The vector potential of the external magnetic field is included by the common manner in the definition of the kinematic momentum. By this means the smooth external fields superimpose into the effective hamiltonian without any change. In all methods of derivation of the effective hamiltonian the translational symmetry of the non-perturbed hamiltonian of the electron in the crystal is essentially used.

Inasmuch as the deformation of the crystal can be described by a smooth function, some authors [5 - 10] proposed to introduce an effective hamiltonian of the electron that depends on the distortion by the phenomenological consideration. In so doing as a rule some unjustified assumption are made. Every so often with an assumption that the kinematic momentum is small there isn't taken into account the dependence of the kinetic energy on the distortion, and the deformation is supposed to generate only the deformation potential, which is proportional to distortion. It is incorrect, because the terms of the hamiltonian that depend on the momentum operator can make a radical change of the spectrum, even though their multipliers are small. Example is provided by the change of the electron states by a weak magnetic field. In the case of a shear deformation in a cubic crystal the deformation potential of the first order is absent by symmetry. Then in the work [7] the amendment proportional to the distortion tensor was inserted into the reciprocal effective mass, but proportionality factor was supposed to be a scalar. In all cited works the introduced effective hamiltonian was used for the solving of the special tasks, and its general characteristics weren't researched.

A great number of works are known, in which the effective wave equation in the approximation of the effective mass has been deduced for the simple model of an electron in the potential field generated by the deformed cubic lattice of short-range ions. This derivation runs into the problem that the difference of the potential energies of the electron in the deformed crystal is a non-local, non-small, and non-smooth function of coordinates. Let us suppose that the

potential energy of the electron has the form:

$$V(\mathbf{x}) = \sum_s V_a(\mathbf{x} - \mathbf{X}_s, \mathbb{W}(\mathbf{x})),$$

where \mathbf{X}_s, \mathbf{x} are the coordinates of the atoms and the electron in the Euler's system of axes, and the function V_a declines rapidly when the first argument increases. It is easily seen that this model incorporates the commonly used models of hard ions and deformable ones. The function $V(\mathbf{x})$ can be represented as the sum of the periodic function and the terms, which are proportional to the powers of the distortion components only if the transformation to the embedded Lagrange's coordinates (1) would be made. If the lattice contains dislocations, that coordinates are discontinuous functions of the Euler's ones, because the displacement field generated by a dislocation has a jump equal to the Burgers vector of this dislocation at some surface bounded by the dislocation line. In other respects the choice of this surface is voluntary, therefore the choice of the Lagrange's coordinates isn't defined unique. It can be made unique if the requirement would be taken that the quantity of the material isn't changed with deformation. The potential energy is a continuous function of the Lagrange's coordinates, because the distortion components are continuous functions, with the exception of the dislocation lines, and their multipliers prove to be periodic functions, which have the full translational symmetry of the ideal lattice. Since the Burgers vector is always one of the vectors of the ideal lattice (a splitted dislocation can be considered as the dislocation with the extended core), then the argument of the periodic function change of the Burgers vector doesn't vary the value of this function. The displacement are not defined on the dislocation line, and the distortion components indefinitely increase, as this line is approached, therefore the transformation to the Lagrange's coordinates and the expansion in terms of the distortion components can't be made in the vicinity of dislocations.

All works use the transformation of the coordinates (1) in one form or another. As a rule, in them there was not taken into account the fact that the area of applicability of this expansion of the potential energy is multiply connected. The other cause of mistakes in the effective hamiltonian derivation in the case of a crystal with dislocations is the neglect of the discontinuity of the transformation (1). If this transformation is used at once to the one-electron Schrödinger equation, as done in the works [11 - 13], then for the continuity of the wave function in the Euler's coordinates special boundary conditions must be defined on the cut surfaces. It makes impossible using the customary method of derivation. The derivation method, which is used in the works [14, 15], can be reduced to the computation of the matrix elements of the one-electron hamiltonian in the representation, the basis of which is constituted by the eigenfunctions for the ideal crystal (the Bloch functions) in which $\mathbf{y}(\mathbf{x})$ is substituted instead the coordinates \mathbf{x} . Using this basis is researched in more detail in the work [16]. In the case of the crystal with dislocations its basis vectors are discontinuous functions, therefore the expansion of the wave functions over them is impossible. These methods can be used only in the case of the compatible deformation. In particular, the transformation of the coordinates (1) is used for the computation of the energy spectrum in uniformly deformed semiconductors in a number of

works summarized in the monograph [17]. However, the extrapolation of these results to the case of non-uniform deformation used in the work [18] is valid only, if the characteristic distance of the deformation variation is considerably greater than the quantity reciprocal to the quasi-momentum modulus. Other attempts to deduce the effective hamiltonian were founded on the representation, the basis of which was constructed from modified Wannier functions [19 - 23]. In these works the fact of small variation of distortion at the distance of the atomic potential influence or of the radius of the Wannier functions was used. This idea was most thoroughly investigated in the work [23]. In so doing it turned out that the diagonalization with respect to the band number with obtaining the one-band effective hamiltonian is impossible.

1.1.2 2.2 . Phenomenological Theory of Effective Hamiltonian

In the section [1.2.3] (here and in what follows in references to the monograph [1] we shall indicate the part number by the second figure, and the section by the third one) the most general effective hamiltonian with the quadratic dispersion law was considered:

$$\widehat{H}^\alpha = \frac{1}{2}\widehat{p}_i\mu_{ij}^\alpha\left(\delta_{jk} + 2A_{jk}^\alpha\right)\widehat{p}_k + V_1 + V_2 + V_3, \quad A_{kl}^\alpha = \frac{1}{2}T_{ijkl}^\alpha w_{ij}. \quad (2)$$

Here μ_{ij}^α are the components of the tensor of the reciprocal effective mass for the band α (in what follows the band index will be omitted). There are taken into account the potential terms not only of the first order V_1 , but also of the second order V_2 , and of the third order V_3 , because for the quadratic dispersion law not only the distortion components, but also the momentum components must be considered as small, and therefore the terms of the third order were considered in the operator of the kinetic energy. This operator can be equivalently rewritten as the quadratic form in new kinematic momentum

$$\widehat{p}_k = -i\hbar\left(\frac{\partial}{\partial x_k} + A_{jk}\frac{\partial}{\partial x_j} + \frac{1}{2}\frac{\partial A_{jk}}{\partial x_j}\right)$$

with the constant coefficients μ_{ij}^α . With using this determination of the kinematic momentum the phenomenological effective hamiltonian can be generalized to the case of the arbitrary dispersion law. In addition it permits to reveal the principal difference between compatible and incompatible deformations. If the tensor \mathbb{A} satisfies the compatibility condition, *i. e.* if it can be represented as the gradient of a continuous and unambiguous vector field \mathbf{u}' , then by the change of the sought function $\psi = \exp\left(\frac{\mathbf{A}\cdot\mathbf{u}}{2}\right)\varphi$, and by the transformation of coordinates $\mathbf{x} = \mathbf{y} - \mathbf{u}'$ the subsidiary terms in the definition of the kinematic momentum can be eliminated. Then the problem is reduced to the common effective equation with a potential. This is like to the elimination of the vector potential of the magnetic field that has zero curl, other than only phase but also modulus of the wave function as well as the coordinates change. If \mathbb{A} is incompatible tensor \mathbf{u}' can't be introduced as a continuous field, and therefore the coordinate change can't be made. Then the solving of the equation with variable multipliers at the derivatives is indispensable. It should be noted that the compatibility of the deformation not necessarily ensures the compatibility of the tensor \mathbb{A} .

1.1.3 2.3. Derivation of Effective Hamiltonian by Introducing of Deformation Basis

In the section [1.2.4] the hamiltonian, which is similar to the phenomenological one, was derived for the simple model described by the hamiltonian of an electron in the potential field generated by the deformed cubic lattice of short-range ions. There was considered the non-degenerated band that has the minimum of energy in the center of the Brillouin zone. With this derivation the limits of the applicability of this hamiltonian were determined and the interpretation of the effective wave function was specified.

The fundamental idea, which permits in the section [1.2.4] to overcome the pointed difficulties in the derivation of the effective hamiltonian in the case of the crystal containing dislocation, is to introduce the new basis in the Hilbert's space of the wave functions, which we shall name the deformation basis.

Let us present shortly the consideration about introducing this basis. The plane waves that can be the basis system of the vectors in the Hilbert's space can be rewritten in the form of the functions, which have the property of Bloch functions for the considered lattice.

$$\Omega^{-\frac{1}{2}} \exp(i\mathbf{K}\mathbf{x}) = \Omega^{-\frac{1}{2}} \exp(i\mathbf{q}\mathbf{x}) \exp(i\mathbf{g}\mathbf{x}) = |\mathbf{q}\mathbf{g}\rangle_B. \quad (3)$$

Here \mathbf{q} is situated in the first Brillouin zone, and \mathbf{g} is a reciprocal lattice vector of the crystal under consideration. Let us name as the deformation basis the set of functions

$$|\mathbf{q}\mathbf{g}\rangle_D = \Omega^{-\frac{1}{2}} \exp(i\mathbf{q}\mathbf{x}) \exp(i\mathbf{g}\mathbf{y}(\mathbf{x})), \quad (4)$$

$\mathbf{y}(\mathbf{x})$ being defined from (1). Therefore $\mathbf{y}(\mathbf{x})$ has the jumps by the Burgers vector. These jumps, when they are multiplied by the reciprocal lattice vector, vary the exponent of power by $2\pi ni$, therefore the functions of the deformation basis are continuous and defined elsewhere except the dislocation lines that construct in the three-dimensional space a set of measure zero. It can be shown that, if the modulus of \mathbf{q} is considerably smaller than the Brillouin zone dimension, the deformation basis functions with different \mathbf{q} and/or \mathbf{g} are approximately orthogonal. The set of the one-electron Bloch eigenfunctions of the hamiltonian in the ideal crystal would be got from the set of the Bloch plane waves (3) by using the unitary matrix $\|B\|$, which is the direct sum over all \mathbf{q} of the unitary matrices $\|B(\mathbf{q})\|$. These matrices connect the Bloch plane waves (3) having coincident \mathbf{q} with the eigenfunctions in the crystal, for which this \mathbf{q} is the quasi-momentum:

$$\Psi_{\alpha\mathbf{q}}(\mathbf{x}) = \sum_{\mathbf{g}} |\mathbf{q}\mathbf{g}\rangle_B B_{\alpha\mathbf{g}}(\mathbf{q}).$$

In Luttinger - Kohn method of the derivation of the effective hamiltonian near to the selected point of the Brillouin zone \mathbf{q}_0 the basis of the representation is got from the Bloch plane waves by the unitary matrix, which is constructed by the same direct sum of the coincident unitary matrices $\|B(\mathbf{q}_0)\|$. Then in the matrix of the hamiltonian of the electron in the ideal crystal and in a smooth external field the block of the elements with small $\mathbf{k} = \mathbf{q} - \mathbf{q}_0$ and $\mathbf{k}' = \mathbf{q}' - \mathbf{q}_0$ can be found, for which the interband elements $H_{\mathbf{k}\alpha, \mathbf{k}'\beta}$ are small and can be eliminated by " $\mathbf{k} \cdot \mathbf{p}$ " perturbation theory. The remaining problem of the diagonalization of the block relating to the single band with respect to the

vector indices \mathbf{k}, \mathbf{k}' can be reduced to the problem of the eigenvalues for the differential operator of the second order that is the effective hamiltonian in the effective mass approximation. Its eigenvalues, which correspond to the smooth eigenfunctions, in sum with $E(\mathbf{q}_0)$ present some part of the energy spectrum of the real hamiltonian, and corresponding wave functions are approximately described by the products of the effective eigenfunctions and $\Psi_{\alpha\mathbf{q}_0}(\mathbf{x})$.

When the effective hamiltonian for the electron in the deformed crystal is derived, the basis for the expansion of the sought function is formed similarly, instead of the Bloch plane waves (3) the functions of the deformation basis (4) are used. The expansion over this basis can determine the wave function only in the multiply connected area, from which the dislocation lines are eliminated. Because in the vicinities of these lines the distortion components are very large, these vicinities must be also eliminated from the consideration, and the boundary conditions for the eigenvalue problem on the surfaces of these "dislocation cores" must be introduced. The power series of the " $\mathbf{k} \cdot \mathbf{p}$ " perturbation theory must be taken in the third order, and then the effective hamiltonian would have the form (2), if the ideal crystal dispersion law has the extremum in the point \mathbf{q}_0 . In so doing the phenomenological constants that are the tensor \mathbb{T} components and the coefficients defining the potential terms are expressed in terms of the matrix elements of certain operators in the representation, which has as the basis the Bloch functions of the ideal crystal. The main result of the derivation of the effective hamiltonian from this model is the elucidation of the facts: the effective equation must be solved with the boundary conditions on the surfaces of dislocation cores, and its solution is the multiplier at the Bloch eigenfunction in the ideal crystal in the band under consideration with quasi-momentum \mathbf{q}_0 , in the periodical factor of which \mathbf{x} is changed for $\mathbf{y}(\mathbf{x})$. The effective hamiltonian has meaning only for a small vicinity of the selected point \mathbf{q}_0 , *i. e.* only smooth eigenfunctions of it that vary no faster than the deformation are of physical sense. If in the point \mathbf{q}_0 the ideal crystal dispersion law has an extremum, then the effective hamiltonian involves only the terms quadratic in the momentum components. The coefficients of these terms are the components of the tensor of the reciprocal effective mass, and depend on coordinates. In a generally case the term linear in momentum will be also involved, it is similar to presence of an external magnetic field that depends on \mathbf{q}_0 . In the case, when N bands have in the point \mathbf{q}_0 the coincident energies, the effective hamiltonian isn't similar to the particle hamiltonian. It is the matrix of the rank N , the elements of which are the operators, and its eigenvector involves N components-functions. The electron wave function is the sum of the N products of these components with the Bloch functions of the corresponding bands, in the periodic multipliers of which \mathbf{x} is changed for $\mathbf{y}(\mathbf{x})$. 2.4. Using of Deformation Basis in Problems of Dynamical Scattering of Electrons and Small Vibrations of Deformed Crystal

It can be shown (see the section [1.2.6]) that the fundamental equations of the theory of the dynamical scattering of electrons in an ideal crystal in the two-rays approximation (see the monograph [24]) can be derived as the effective wave equation for the reciprocal space point that is situated on the Brillouin zone boundary. That can be made by some modification of the Luttinger -

Kohn method. The equations of the scattering by a deformed crystal can be derived through the use of the deformation basis functions instead the plane waves in this modified method. They coincide with the well known Takagi's equations (see the work [25]), which have been derived from the less rigorous considerations, but their solutions describe the amplitudes of the deformation basis functions rather than of the plane waves.

The problem of the eigentones of a deformed crystal that is considered in the section [1.2.5] closely resembles the electron problem described above. Let us choose the displacements of atoms from the sites of the deformed lattice as coordinates, on which the potential energy of the crystal depends. Then zero displacements correspond to the minimum of the potential energy, though not absolute one. The set of motion equations is got by the power series expansion of the potential energy in the second order, and describes small vibrations of atoms about the equilibrium positions that constitute the deformed lattice. Let us search the solution of this set in the form:

$$\mathbf{u}^\nu(\mathbf{X}_0^\nu, t) = \mathbf{U}(\mathbf{X}_0^\nu) \exp(i\mathbf{k}\mathbf{X}_0^\nu) (1 + \frac{1}{2}w_{jj}^\nu) \cos \omega t.$$

Here the Greek indices number the lattice sites, \mathbf{X}_0^ν are the coordinates of these displaced sites. It can be seen that this solution differs from the common wave solution in the perfect crystal by the dependence on the site coordinates of the vector describing the magnitude and polarization of vibrations. This is true, because the translation nonexists that retains the lattice transferring its sites one into other. If it is granted that the values of $\mathbf{U}(\mathbf{X}_0^\nu)$ little differ in the neighboring sites, this vector can be described by a smooth function of the continual argument. Then the set of the three differential equations, *i. e.* the matrix eigenvalue problem, for the components of this vector can be obtained. These eigenvalues define the squared eigentone frequencies, and three frequencies correspond to any wave vector. The corresponding eigentones are the plane waves with modulated magnitudes and polarizations. In an ideal crystal in the symmetrical point of the Brillouin zone the vibrations can be presented as the longitudinal and two transverse waves with coinciding frequencies of the transverse ones. Then in the deformed crystal also one equation can be separated out of the set, which describes the mainly longitudinal vibrations, which have weakly modulated polarization. In transverse waves the vibration polarizations would strongly depend on coordinates, and the space beatings would take place. The magnitude modulation can be deep, *i. e.* the local, but sufficiently spacious can exist.

1.2 3. Electron States in Deformed Crystal

1.2.1 3.1. General Consideration about Electron States in Deformed Crystal

The effective one-electron hamiltonian derivation is only the first necessary step to the creation of the electron phenomena theory. In principle, the full set of the eigenstates and the energy spectrum of the electron in the band can be obtained by selecting some set of points in the Brillouin zone of the non-deformed crystal,

deriving the effective hamiltonian in these points, and solving the eigenvalue problems. Each eigenstate obtained by this way will be characterized by not only the band number (if the band in this point is non-degenerated in the ideal crystal) and the energy, but also by the Brillouin zone point, in which it has been obtained. It is clear that in so doing this point isn't an exact quantum number. But the making of this description demands exact knowledge of the distortion tensor and the boundary conditions on the dislocation core surfaces. In the most interesting cases the distortion field and the boundary conditions can be neither well measured nor reproduced in the predetermined view. Therefore only the observable quantities that are defined by the statistical characteristics of the ensemble of possible values of the distortion and boundary conditions have the physical sense. The theory of this type was made, *e. g.*, for the kinematic scattering of X-rays in the monograph [26]. Some results in the electron theory with taking into account only the deformation potential was obtained by I. M. Lifshitz (see the review [27]). The dependence the kinetic energy parameters (*e. g.* the effective mass tensor components) on coordinates can lead in addition to transformations in the one-electron state system that are not evident at present time. The Hamilton's equations that can be derived from the effective hamiltonian quadratic in the momentum components by the reversion of the correspondence principle are non-linear, because the derivatives of the classic hamiltonian with respect to coordinates are the quadratic functions of the momentum components. In most cases they are very complicated and supposedly non-integrable. As of now the question about characteristics of the quantum system that corresponds to the classical one, the motion of which is chaotic in the considerable proportion of the phase volume, is insufficiently studied.

1.2.2 3.2. Localized States in Potential Well Close to Rectilinear Edge Dislocation

Some cases of the electron states in defined distortion field have been considered elsewhere and are described in the third chapter of the monograph [1]. A number of works was devoted to localized electron states in the field of the deformation potential that is proportional to the dilatation generated by the rectilinear edge dislocation in an isotropic medium. In the work [28] it is shown that the state energies, which are close to the continuous spectrum, are approximately inversely proportional to their number in the sequence arranged in the order of increasing. In the works [29], and [30] the energy of the ground state was obtained by the variational method. In the section [1.3.2] these results are improved by the proposed modification of the variational method. The considered hamiltonian is represented as the sum of two terms $\hat{H} = \hat{H}_0 + \hat{H}_1$ so that eigenfunctions of \hat{H}_0 can be found. These eigenfunctions are used as a trial functions in the standard variational procedure. This decomposition is defined by some parameters that are calculated further through the minimization of the expectation value \hat{H} in the ground state of \hat{H}_0 . This expectation value has the form of the expression of the ground state energy \hat{H} correct in the first order of

the perturbation theory, in which \widehat{H}_1 is considered as a perturbation. There can be calculated the values of the expansion parameters of this perturbation theory $\frac{\langle 0|\widehat{H}_1|m\rangle}{E_0-E_m}$, where $\langle 0|, |m\rangle, E_0, E_m$ are the eigenfunctions and corresponding eigenvalues of the operator \widehat{H}_0 with the values of the decomposition parameters obtained by minimization $\langle 0|\widehat{H}|0\rangle$. If these parameters of the perturbation theory are smaller than unity, the obtained value of the ground-state energy can be improved by calculating the amendment of the second order, which is always negative. The function of the zero or the first order can be considered as the approximate expression for the ground-state eigenfunction, and the energies and eigenfunctions of some low-lying excited states can be calculated. It is apparent that this method is inapplicable, when the distance between neighboring eigenvalues of the hamiltonian \widehat{H}_0 is small. It would be, in particular, close to the bound between discrete and continuous parts of the spectrum. When the problem electron ground-state in the field of the deformation potential of the edge dislocation is considered, it is found that the requirement of the eigenfunction continuity leads to the necessity of its going to zero on the dislocation line. This is an acceptable boundary condition for the effective wave function, because then the indeterminacy of the real wave function on the dislocation line disappears. But the extrapolation of the deformation potential to the vicinity of the dislocation line is obviously incorrect, because it is not only very large in this vicinity, but also is indeterminate on the dislocation line.

3.3. Integrable Schrödinger Equation with Effective Mass Depending on Coordinates

Of particular interest is the effective wave equation in the case of distortion field generated by a rectilinear screw dislocation in an isotropic medium. The deformation potential of the first order in distortion in this case is absent by symmetry and the effective mass depending on coordinates has a dominant role. As discussed earlier precisely this kind of perturbation is specific for the deformation effect. In this case the variables in the equation can be disjointed in cylindric coordinate system. It permits to integrate the equation completely, and to study the obtained solutions. That was made partially in the works [28], [29]. Inasmuch the analysis of this equation enables to consider some new characteristics of the effective wave equation, let us dwell on it in detail.

In this case the hamiltonian (2) leads to the equation

$$-\frac{\hbar^2}{2}\mu\left[\nabla^2 + \frac{b}{\pi(x_1^2+x_2^2)}T\left(-x_2\frac{\partial}{\partial x_1} + x_1\frac{\partial}{\partial x_2}\right)\frac{\partial}{\partial x_3}\right]\Psi + \frac{v}{x_1^2+x_2^2}\Psi = (E - E_\alpha)\Psi. \quad (1)$$

Here μ is the reciprocal effective mass and E_α is the energy in the center of the Brillouin zone in the band α , the constant T is the shear component of the tensor \mathbb{T} , which is supposed to have the symmetry of isotropic medium, v is the constant of the deformation potential of the second order, the deformation potentials of the first and the third orders are zero by symmetry. Let us divide this equation by $\hbar^2\mu$, transform it to the cylindrical coordinates and substitute $\Psi = \exp(ik_3z)U(\rho, \varphi)$. We obtain the equation:

$$-\frac{1}{2}\left(\frac{\partial^2 U}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial U}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 U}{\partial \varphi^2}\right) - \frac{i\zeta}{\rho^2}\frac{\partial U}{\partial \varphi} + \frac{\xi}{\rho^2}U = \sigma_1\frac{\varepsilon^2}{2}U.$$

Here notes are introduced:

$$\frac{bTk_3}{\pi} = \zeta, \quad \frac{v}{\hbar^2\mu} = \xi, \quad \text{sign}(E - E_\alpha) = \sigma_1, \quad \left| E - \frac{\hbar^2}{2}\mu k_3^2 - E_\alpha \right| = \frac{\hbar^2}{2}\mu\varepsilon^2.$$
 This equation describes also the amplitude of eigentones in a body centered crystal with the screw dislocation directed along the axis [111], when its polarization is directed mainly parallel to the dislocation and also the wave vector. It is significant that ζ can have positive or negative values depending on to be aligned the Burgers vector either with the quasi-momentum component k_3 or opposing it. This component is a good quantum number, and can assume any values within the boundaries of the Brillouin zone, because the crystal with the rectilinear dislocation retains the translational symmetry in the dislocation direction. Then the equation can be generalized to considering it as the Schrödinger equation for the hamiltonian, which is got by expansion of any dispersion law in terms of small transversal components of quasi-momentum with any determined k_3 . In so doing in the determination of ζ instead of the multiplier k_3 an odd function of k_3 appears, which can be non-monotonous in particular.

The solution of this equation have the form:

$$U = \exp(im\varphi) Z_\tau(\rho\varepsilon\sqrt{\sigma_1}),$$

where m is a natural number, $Z_\tau(z)$ is a cylindrical function with the index $\tau = \sqrt{\sigma_2|m^2 + 2\zeta m + 2\xi|}$, $\sigma_2 = \text{sign}(m^2 + 2\zeta m + 2\xi)$. The boundary condition on the dislocation core in the works [28], [29] is supposed in the form of the demand of the continuity of the solutions in the total space. For the fulfillment of this condition there is supposed $\sigma_1 = \sigma_2 = 1$. In [1.3.3] the logarithmic derivative of the solution on the dislocation core bound can assume any real values depending on the form of the wave function in the dislocation core including the infinite value. Then with the values $\sigma_1 = 1$, $\sigma_2 = -1$ and $\sigma_1 = -1$, $\sigma_2 = -1$ the boundary condition can also be fulfilled. The equation has been researched by the version of the JWKB method proposed in the monograph [30]. This allows considering the effect of the boundary condition and the correspondence between the characteristics of the equation solutions and of the motion of the classical particle, the hamiltonian of which is obtained without using the correspondence principle, which is non-founded for the effective hamiltonian, and is inapplicable in the case of the crystal vibrations. In both cases, when $\sigma_1 = 1$, the solutions belong to the continuous spectrum. By them the function describing the scattering of an electron by the screw dislocation can be constructed. It was made in the works [28], [29] as well, but in the section [1.3.3] there is first pointed that, if for some values of k_3 would be $\sigma_2 = -1$, the scattering by attraction replaces scattering by repulsion, and the dislocation core must play a great part. The other essential singularity, which also is not be noted elsewhere, is that the scattering by the screw dislocation is non-symmetrical with respect to the plane, in which the dislocation line and the electron quasi-momentum are situated.

1.2.3 3.4. "Kinetic Well" in Classic and Quantum Problems

When $\sigma_1 = -1$, $\sigma_2 = -1$, the energy of the motion in the transversal plane takes only discrete negative values, and the corresponding states are localized. This is an example of the new type of the localization that can originate from a special dependence of the effective mass on coordinates. Unlike a classical particle, a band electron can have negative kinetic energy (a hole), if the dispersion law has a maximum in the Brillouin zone center. In the deformed crystal, when the dispersion law depends on coordinates, the sign of the kinetic energy may turn out different in various areas of the crystal. The electron, which has the negative energy and non-zero momentum, moves, but it can't go out to the area, in which its kinetic energy shall be positive. We can say that it is situated in a "kinetic well" distinguished from the ordinary potential one. In a similar manner it may be, when the summand of the kinetic energy, which is an independent constant of motion, has different sign in various areas of the crystal. In the section [1.3.3] there is obtained the dependence of the discrete eigenvalues arranged in order of increasing on their number. Close to the bound between discrete and continuous spectra their absolute values constitute a decreasing geometric progression.

When the momentum component operators in the effective hamiltonian are changed for c -quantities, the quasi-hamiltonian of the classic particle would be obtained. It can't be contended that the phase trajectory of this particle describes the variation with time of the averaged characteristics of the electron wave packet. But there is no question that the properties of the Hamilton's equations are connected with the properties of the Schrödinger equation, although this connection isn't studied adequately. In section [1.3.4] the motion of this classic particle is considered in the case of a screw dislocation with the condition of mirror-like reflection from the cylindric dislocation core. The motion equations in this case can be exactly solved. At some value of the hamiltonian parameters there is an area of the phase space in which the motion in the plane perpendicular to the dislocation is finite and conventionally-periodical. By using Bohr - Sommerfeld quantization rules the same spectrum of the quasi-classical energy levels can be obtained. When a small regular perturbation is added into the hamiltonian, an area of a chaotic motion arises in the vicinity of the separatrix that delimits the areas of finite and infinite motions. What are the characteristics of the quantum system that correspond to this feature of its classical analogue is not clarified presently.

An other example of the kinetic well is considered by using the classical analogue in the section [1.3.5]. If an edge rectilinear dislocation in an elastically isotropic crystal with the Poisson constant equal 0.5 is considered, the deformation potential in the effective hamiltonian is equal to zero. The disturbance of the deformation and the change of the lattice topology in this case are described by the dependence of the effective mass on coordinates. The solving of Schrödinger equation in this case has not met with success, but the corresponding Hamilton's equations can be analyzed by the qualitative investigations and by the numerical integration. It is found that closely to dislocation and symmetrically about it the two bounded domains exist, in which the effective mass

of transversal motion is negative. Therefore the motion of a particle in these domain must be finite. The motion integrals other than energy supposedly don't exist, and because of this the quasi-classical quantization can't be performed.

1.2.4 3.5. One-Electron States in Deformed Crystal in Magnetic Field

One-electron states in a deformed crystal in the magnetic field were researched by the quasi-classical quantization the motion of the corresponding classical particle. If the hamiltonian parameters to a good approximation can be supposed to be constant in the area that contains the electron trajectory, this trajectory is a helical line with the axis directed along the magnetic field. The projection of this trajectory on the plane perpendicular to the magnetic field is an ellipse, and this motion can be quantized by the Bohr - Sommerfeld quantization rules with the discrete equidistant energy spectrum as a result. As usually (see the monograph [31]), there is supposed in the section [1.3.6] that the energetic spectrum can be described as the superposition of the equidistant sequences, zero points of which are determined by local values of the potential energy, if the potential is a smooth function of coordinates, so that it is little varied within the limits of the Larmor's orbits under considered energies. More recently (unpublished) the author has concluded that this supposition that means the electron stationary state to be localized close to the corresponding classical orbit is incorrect. The Larmor's radius determines the wave function localization only in a direction perpendicular to some line that can have a length of the order of the dimension of the all potential well, in which the electron is situated. This line is determined by the choice of the coordinate system and its origin, and therefore this localization has a physical sense only, when the space inhomogeneity determines this choice. In the case of the solving in the rectangular coordinates, *e. g.*, (see the monograph [32]) there are straight lines $y = y_0$, where y_0 are the eigenvalues of the orbit center operator that has a discrete spectrum. In so doing the orbit center abscissa remains to be uncertain. When the solution is taken in the polar coordinate system, the state is characterized by the orbit center distance from the coordinates origin that can take the discrete values, but the center azimuth remains to be uncertain. This uncertainty is peculiar to this problem, because the operators of the coordinates of the orbit center commute with the hamiltonian, but don't commute with one another. The solutions of the time Schrödinger equation that are the Gaussian wave packets, which move at the fixed in the space classical orbits with the minimally uncertain centers, what are called as coherent states, are not the hamiltonian eigenfunctions. The author has obtained the exact solution of the quantum-mechanical problem about an electron in the uniform magnetic field and the step potential (unpublished) and showed that this energy spectrum doesn't coincide with one obtained by the quantization of the motion integral of the corresponding classical problem. In so doing the largest differences are obtained at large quantum numbers. Therefore the question about the thermodynamic and galvanomagnetic characteristics of the electron gas in the nonuniform potential field requires further investigation.

It appears to be evident that the trajectory of the classical particle, the hamiltonian of which is obtained from the effective hamiltonian with the uniform magnetic field, must be unlocked similar to the Burgers contour, when this particle envelopes the dislocation line. In the section [1.3.6] it is justified by the solving of the corresponding motion equations. In the case of the screw dislocation parallel to the magnetic field this doesn't break the locking of the trajectory projection on the plane perpendicular to the field, and the motion integrals: the angular momentum with respect to the dislocation line, and the radial component of the action - can be quantized. If the dislocation core radius would be considered zero, the transversal motion hamiltonian coincide with the electron hamiltonian in the uniform magnetic field, and the field of the magnetic string, *i. e.* infinitely thin solenoid, the flux of which is proportional to the Burgers vector and to the longitudinal momentum. The exact solution of the corresponding quantum-mechanical problem is known (see the work [33]). Its spectrum coincides with one that obtained by the quasi-classical quantization. In the case of several screw dislocations or magnetic strings the axial symmetry is destroyed, but the classical problem retains to be solvable for the trajectories, which don't cross the dislocation lines. On the base of this solution a hypothesis about the electron energy spectrum in this field was suggested in the section [1.3.6]. But recently (unpublished) the author has obtained the exact solution of this quantum-mechanical problem, from which follows that this hypothesis is incorrect. This problem also requires further investigation.4. Many-Electron Phenomena in Deformed Crystal

1.2.5 4.1. Electrical Field in Deformed Conductors

When the effective hamiltonian was derived in the section [1.2.4], it was supposed that the effect of the lattice atoms on the electron goes to zero at a distance of several lattice constants. If other electrons are in the crystal, and all or some part of atoms are ions, they generate the electric field that can't be supposed proportional to the deformation in the point under consideration. In the section [1.4.1] in the self-consistent field approximation the equation for the electrostatic potential generated by the all electrons and ions of the deformed crystal is derived. This potential must be included into the one-electron effective hamiltonian.

Let us describe shortly this derivation. The smooth component of the nonuniform density of the ion charge is proportional to dilatation, *i. e.* the trace of the distortion tensor. The nonuniform electron density is formed self-consistently, *i. e.* so that the flow, which should be generated by the electric field, is entirely compensated by the diffusion flow generated by the electron density heterogeneity. The total electric charge density is a smooth function and generates a smooth self-consistent electric field. The potential of this field can be taken away from the potential energy of the one-electron Schrödinger equation. Then the residual is the short-range ion potential that was considered in the section [1.2.4]. It is not periodic in the deformed crystal. If in the Lagrange's curvilinear coordinates the periodic term would be detached,

the residual term will be small, because it is proportional to distortion, but non-smooth function of coordinates. This residual term leads to the smooth deformation potential in the effective hamiltonian. The deducted potential of the self-consistent field as the smooth function can be added to the potential energy of this hamiltonian. Then the electron density amendment depending on the potential of this self-consistent field would be obtained by the perturbation theory. On the other hand, this potential is related with the density of electrons and ions by the Poisson's equation. As a result the closed equation for the self-consistent field potential would be obtained. Generally it is integro-differential equation. In the case, *e. g.*, of non-degenerated electron gas it has a form:

$$\Delta\varphi - \lambda^2\varphi + \frac{\lambda^2}{V} \int_V \varphi dV = -\frac{1}{\varepsilon_0}\Xi(\mathbf{r}) + \frac{1}{\varepsilon_0 V} \int_V \Xi(\mathbf{r}) dV - \frac{q}{\varepsilon_0}.$$

Here

$$\Xi(\mathbf{r}) = en_0 \left[\frac{1}{2} \mu_{ij} T_{klji} w_{kl} + \frac{U}{kT} + w_l(\mathbf{r}) \right]$$

is the inoculating heterogeneity of the charge density that is given by the trace of the tensor of the reciprocal effective mass (see formula (2)), the deformation potential U , and the heterogeneity of the positive charge density proportional to the dilatation; λ is the reciprocal of the shielding radius; V is the crystal volume; q is the crystal charge; e is the modulus of the electron charge; n_0 is the electron density in the non-deformed crystal. The solution of this equation must be got in the all volume the conductor and be joined on the bound with the solution of the Poisson's equation for the surroundings. In metals, *i. e.* in a conductor with degenerated electron gas, instead of the multiplying by λ^2 the integral operator with the core defined by metal electron characteristics appears. In the case of a point inoculating charge it leads to the well-known shielding charge density oscillations. These equations in the conducting bodies play the same role as the Poisson's equation in the non-conducting ones. They form a new method in the electrostatic of continuous mediums, in which the electric field in the conductor isn't supposed to be zero a priori. The solution can always be found as the sum of the partial solution of the nonuniform equation with zero boundary conditions and the general solution of the uniform equation containing the voluntary constants, with help of which the boundary conditions can be satisfied. As an example, the problem is considered about the electric field within the thickness of the hollow cylinder and beyond it, when the cylinder is deformed as if an edge dislocation with the macroscopic Burgers vector were situated on its axis. The solution shows that this cylinder generates the field similar to the dipole field, which can be not very small. The equations can also be used for the uniform, but bounded conductor with $\Xi(\mathbf{r}) = 0$ in an external field. For example, in the case of a conductor with the non-degenerated electron gas the solution of the corresponding equation describes the exponential decreasing of the external field with moving from the bound into the thickness. The approximate solution of the problem about an uniform plate with the degenerated electron gas in the uniform external field perpendicular to it shows that the field in the plate aside from a term exponentially decreasing with moving off the surface contains a small oscillating amendment that has the maximum in the center of the plate.

1.2.6 4.2. Heterogeneous Kinetic Coefficient in Deformed Conductor

In the next section [1.4.2] the transport phenomena in the deformed conductor are studied. In the theory of the transport phenomena an incorrect method was in general use, in which dislocations were considered similarly to point scattering centers. In fact it is obvious that the scattering by the long-range fields can't be accounted by the Boltzmann integral. It is incorrect also to consider the scattering by several dislocations as the sum of the effects from single dislocations. In most important cases the method by S. I. Pecar is applicable, in which it is supposed that other scatterers cause so small distance of the electron free path that the deformation generated by the dislocation can be considered on this distance as uniform. Then let us determine the kinetic coefficients in any uniformly deformed volume with the dimensions much larger than the distance of the electron free path, and next solve the problems for the non-uniformly conducting bodies. In the works using this method the symmetrical case, when the kinetic coefficients are scalars, was commonly considered. Furthermore, there was taken into account only variation of the electron density that satisfies to the quasi-neutral requirement. As result in the deformed conductor the conductivity also would remain scalar, though it would depend on coordinates. In the section [1.4.2] the anisotropy of the effective mass generated by the uniform shear deformation is also taken into account. By solving the kinetic equation the tensor kinetic coefficients are obtained that can explain some experimental effects. As an example the flowing of the electric current parallel to the screw dislocation must be accompanied by the flowing of the circular currents that envelops its axis, and consequently by the axial component of the magnetic field.

1.2.7 4.3. Transition to Superconducting State and Current in Deformed Superconductors

The influence of the deformation on various phenomena in superconductors is considered in the sections [1.4.3], and [1.4.4] on the base of plausible or experimentally confirmed phenomenological suppositions. To cite an example, on the base of the known fact of the dependence of the superconducting transition temperature on the lattice hydrostatic compression, a supposition is made that in the superconductor with smoothly non-uniform dilatation a field of the local transition temperature $T_C(\mathbf{r})$ can be introduced. We can consider this field as smooth, if the correlation radius of the order parameter fluctuations determined by the modulus of the difference $|T - T_C(\mathbf{r})|$ is (at various temperatures in the various areas) much smaller than the characteristic distance of the field variation. Then in the areas in which the difference $T - T_C(\mathbf{r}) < 0$ and is sufficiently large modulo the ordered regions should appear. The appearance of this region close to an edge dislocation predicted firstly in the work [34] is studied in more detail in the section [1.4.3]. The appearance of the ordered region close to a screw dislocation and the influence of the magnetic field on this phenomenon

is also described. The general theory of phase transitions of the second kind in systems heterogeneous in large scale, which was developed in works by M. A. Krivoglaz and the author (see the review [35]) holds that the appearance of these ordered regions isn't the true phase transition. The ordered regions would form a framework piercing through all the superconductor, but they are broken up into domains with random values of the order parameter phase by zones of the phase slip. In these zones the modulus of the order parameter approaches to zero and thereafter increases anew to the equilibrium value. The true superconductivity in this framework shall also be absent so long as the averaged domain length will be smaller than the averaged length of the superconducting regions between the points of their intersections with other ones. Only when this condition will be satisfied, it will be possible to pass over the framework of the superconducting regions at any distance without intersection of any boundary of the phase slip, *i. e.* in the system the long-range order will appear.

Some effects, which follow from the supposition that the deformation of the superconductor can make it anisotropic, are considered. In so doing the proportionality coefficient \mathbb{P} in the equation for the superconduction current density

$$\mathbf{j} = \mathbb{P} n_s (\hbar \nabla \Phi - \frac{2e}{c} \mathbf{A})$$

becomes a tensor of the second rank that depends on coordinates. Here n_s is the density of the superconducting electrons, Φ is the order parameter phase, \mathbf{A} is the magnetic field vector potential. After eliminating $\nabla \Phi$ with the help of the operation "curl" and \mathbf{A} by the use of the Maxwell's equations the closed differential equation for \mathbf{j} is obtained. Its solution in the case, when \mathbb{P} depends linearly on the deformation generated in the hollow cylinder by the screw dislocation at its axis describes the paradoxical effect: the longitudinal transport current parallel to the screw dislocation is accompanied by the circular current that envelopes the dislocation. This current flows close to the outer surface of the cylinder and generates the longitudinal magnetic field, which increases deep into the superconductor and passes a maximum at the distance the London's length.

1.2.8 4.4. Abrikosov's Vortex in Anisotropic and Deformed Superconductor

The deformation amendments to the tensor \mathbb{P} and the superconducting transition temperature cause the interaction of an Abrikosov's vortex with the deformation field. If the deformation varies on the distance, which is larger than the London's length the studying of its effect on the Abrikosov's vortex can be reduced to the consideration of the energy of this vortex fragment in a uniformly deformed superconductor. The high- T_C -superconductors, as a rule, are highly anisotropic in non-deformed condition as well. Therefore the characteristics of the Abrikosov's vortex in the anisotropic superconductor are very interesting.

The behavior of a straight Abrikosov's vortex in an anisotropic uniaxial London's superconductor is studied in [1.4.4]. Analytical expressions are derived that approximately describe the magnetic field in three regions: the asymptotic

region, where the distance r from the vortex line is greater than $\lambda\Gamma$ (λ is the London's length and Γ is the anisotropy constant), the intermediate region $\lambda < r < \lambda\Gamma$, and the region $r < \lambda$. It is found that, when the anisotropy is large, in the intermediate region the component of the magnetic field along the vortex line changes its sign for a certain interval of angles between the vortex line and the anisotropy axis. Because of this the interaction of parallel vortices, whose plane is parallel to the anisotropy axis, has a minimum and a maximum. This means that numerous metastable vortex lattices can exist. Additional terms in the vortex self-energy are obtained, and although they are smaller than the leading logarithmic term, they display a different dependence on the angle between the vortex line and the anisotropy axis. Furthermore in the section [1.4.4] it is shown that the common opinion about increasing the Abrikosov's vortex specific energy in bending is incorrect. Because of attraction of the parallel currents forming an Abrikosov's vortex the vortex energy per unit length decreases, while bending the vortex, by a quantity proportional to the square of the curvature. Solving the London's equation in an approximation allowing for this effect makes it possible to calculate the energy of an Abrikosov's vortex, which has the form of a helix, whose radius and pitch are much larger than the correlation length, whose curvature is small compared to the reciprocal London's length, and whose slope in relation to an axis coinciding with the direction, in which vortex energy is the highest, is also small. When the anisotropy is large, which is characteristic of high- T_C -superconductors, the energy of such Abrikosov's vortex is lower than of a straight Abrikosov's vortex. Certain consequences of the fact that the Abrikosov's vortices in a high- T_C -superconductor are helical are discussed. Among these is a phase transition that breaks symmetry between Abrikosov's vortices shaped like right- and left-hand helices in relation to the magnetic field.

The interaction of Abrikosov's vortex with dislocations perpendicular to Cu-O layers in high- T_C -superconductor at distances greater than the characteristic dimensions of the vortex and of the dislocation is discussed. This interaction is caused by local changes of the order parameter with the dilatation, as well as of the direction of the anisotropy axis with the shear deformation. It is shown that such interaction does not produce any centers of pinning, but facilitates the attraction of a vortex to the dislocation core. And if a thermal fluctuation will throw the vortex over the dislocation core, this interaction will repel the vortex from the dislocation. Coiling of the vortex around a screw dislocation core in the direction of helicoid formed by Cu-O layers in a crystal with a dislocation can be a pinning center.

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